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Scientific and Technical Information

SEARCH REQUEST

Requester's Full Name: Robinson, Binta ExamArt Unit: 1625Phone Number: 2-0692Serial Number: 10583635Location (Bldg/Room#): 4470 (Mailbox #):

Results Format Preferred (circle): PAPER DISK

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention:

Process for the manufacture of 2,3-dichloropyridine

Inventors (please provide full names):

Rafael Shapiro

Earliest Priority Date:

1/23/04

Search Topics

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequencer Searcher Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

See claims 1-27

=> file registry

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10/583635

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STRUCTURE FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8
DICTIONARY FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8

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=> file zcaplus

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FILE COVERS 1907 - 6 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 5 Mar 2009 (20090305/ED)

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate
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'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L64

L2 9 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (1317-38-0/BI OR
2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9

L4 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L2 AND NC5/ES

L5 5 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L4 NOT L3

L9 572 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (462-08-8/CRN OR
6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CRN)

10/583635

N)

L11 575 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L9 OR L5

L23 16 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON C5H3CL2N/MF

L26 109 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (1001003-85-5/CRN OR
1001003-86-6/CRN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR
1001003-91-3/CRN OR 1001003-97-9/CRN OR 16110-09-1/CRN OR
2402-77-9/CRN OR 2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/C
RN OR 26452-80-2/CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR
851516-88-6/CRN OR 98136-41-5/CRN)

L27 125 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L23 OR L26

L28 571 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (C5H5CLN2.CLH/MF OR
C5H5CLN2/MF OR C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)

L29 151 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L28 AND NC5/ES

L42 721 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L11 OR L29

L43 721 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L42 AND NC5/ES

L62 866 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON SHAPIRO R?/AU

L64 4 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON (L27 OR L43) AND L62

=> d ibib abs hitstr L64 1-4

L64 ANSWER 1 OF 4 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:696875 ZCAPLUS Full-text

DOCUMENT NUMBER: 143:155307

TITLE: Process for the manufacture of 2,3-dichloropyridine

INVENTOR(S): Shapiro, Rafael

PATENT ASSIGNEE(S): E.I. Dupont de Nemours and Company, USA

SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005070888	A2	20050804	WO 2005-US2462	20050121
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005206576	A1	20050804	AU 2005-206576	20050121
CA 2553850	A1	20050804	CA 2005-2553850	20050121
EP 1706381	A2	20061004	EP 2005-712075	20050121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS, YU				
CN 1910152	A	20070207	CN 2005-80002691	20050121
BR 2005006502	A	20070227	BR 2005-6502	20050121
JP 2007523065	T	20070816	JP 2006-551437	20050121
US 20070161797	A1	20070712	US 2006-583635	20060620
IN 2006DN03640	A	20070824	IN 2006-DN3640	20060623
MX 2006008208	A	20060831	MX 2006-8208	20060719
KR 2006130618	A	20061219	KR 2006-714736	20060721

10/583635

PRIORITY APPLN. INFO.:

US 2004-539068P

P 20040123

WO 2005-US2462

W 20050121

OTHER SOURCE(S): CASREACT 143:155307

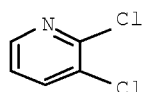
AB A method for preparing 2,3-dichloropyridine is disclosed in which 3-amino-2-chloropyridine is contacted with an alkali metal nitrite in the presence of aqueous hydrochloric acid to form a diazonium salt; and the diazonium salt is subsequently decomposed in the presence of copper catalyst wherein at least about 50% of the copper is the copper(II) oxidation state.

IT 2402-77-9P, 2,3-Dichloropyridine

RL: IMF (Industrial manufacture); PREP (Preparation)
(process for the manufacture of 2,3-dichloropyridine)

RN 2402-77-9 ZCAPLUS

CN Pyridine, 2,3-dichloro- (CA INDEX NAME)

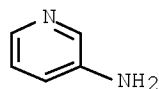


IT 73074-20-1P, 3-Aminopyridine hydrochloride 94770-75-9P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT
(Reactant or reagent)
(process for the manufacture of 2,3-dichloropyridine)

RN 73074-20-1 ZCAPLUS

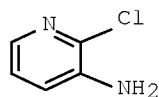
CN 3-Pyridinamine, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 94770-75-9 ZCAPLUS

CN 3-Pyridinamine, 2-chloro-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

IT 98-92-0, Nicotinamide 462-08-8, 3-Aminopyridine

6298-19-7, 3-Amino-2-chloropyridine

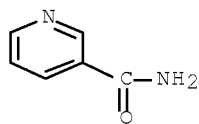
RL: RCT (Reactant); RACT (Reactant or reagent)

(process for the manufacture of 2,3-dichloropyridine)

RN 98-92-0 ZCAPLUS

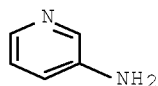
10/583635

CN 3-Pyridinecarboxamide (CA INDEX NAME)



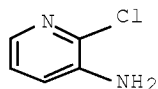
RN 462-08-8 ZCAPLUS

CN 3-Pyridinamine (CA INDEX NAME)



RN 6298-19-7 ZCAPLUS

CN 3-Pyridinamine, 2-chloro- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 2 OF 4 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2000:301510 ZCAPLUS Full-text

DOCUMENT NUMBER: 133:104837

TITLE: Using Intelligent/Random Library Screening To Design Focused Libraries for the Optimization of Homogeneous Catalysts: Ullmann Ether Formation

AUTHOR(S): Fagan, Paul J.; Hauptman, Elisabeth; Shapiro, Rafael; Casalnuovo, Albert

CORPORATE SOURCE: Central Research and Development Department, The Dupont Company, Wilmington, DE, 19880-0328, USA

SOURCE: Journal of the American Chemical Society (2000), 122(21), 5043-5051

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

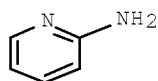
OTHER SOURCE(S): CASREACT 133:104837

AB A 96-member pyridine library consisting of both rationally chosen and random members was used to screen Ullmann ether forming reactions. The reaction of 2-bromo-4,6-dimethylaniline and other substrates with a variety of alkoxides was studied under different conditions with the aid of an automated liquid handler. From the results of the 96-member library screening, a structure activity profile was determined which led to the design of smaller focused

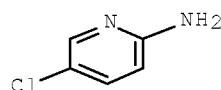
10/583635

ligand libraries. The focused libraries produced a higher frequency of hits compared to the original 96-member library. Some of the more effective ligands discovered in this work are generally useful for alkoxylation of a variety of substrates, and also functioned in intramol. ether forming reactions. This work demonstrates for homogeneous catalysis the analogy to the pharmacol. model of drug discovery. By using a large library to screen for a lead compound followed by screening the diversity space closest to the lead, a larger fraction of increased performance ligands was discovered.

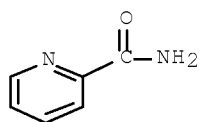
IT 504-29-0, 2-Aminopyridine 1072-98-6,
2-Amino-5-chloropyridine 1452-77-3, Picolinamide
1453-82-3, Isonicotinamide 34813-97-3
RL: CAT (Catalyst use); USES (Uses)
(optimization of pyridine ligand components for catalytic Ullmann
alkoxylation)
RN 504-29-0 ZCAPLUS
CN 2-Pyridinamine (CA INDEX NAME)



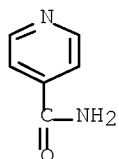
RN 1072-98-6 ZCAPLUS
CN 2-Pyridinamine, 5-chloro- (CA INDEX NAME)



RN 1452-77-3 ZCAPLUS
CN 2-Pyridinecarboxamide (CA INDEX NAME)

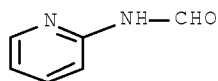


RN 1453-82-3 ZCAPLUS
CN 4-Pyridinecarboxamide (CA INDEX NAME)



10/583635

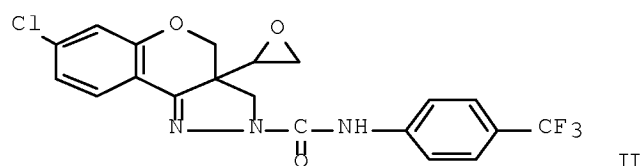
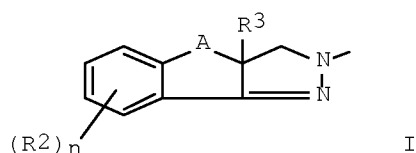
RN 34813-97-3 ZCAPLUS
CN Formamide, N-2-pyridinyl- (CA INDEX NAME)



REFERENCE COUNT: 112 THERE ARE 112 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L64 ANSWER 3 OF 4 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1996:35002 ZCAPLUS Full-text
DOCUMENT NUMBER: 124:202246
ORIGINAL REFERENCE NO.: 124:37393a,37396a
TITLE: Arthropodicidal pyrazolines, pyrazolidines and
hydrazines
INVENTOR(S): Harrison, Charles R.; Lett, Renee M.; Mccann, Stephen
F.; Shapiro, Rafael; Stevenson, Thomas M.
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: U.S., 64 pp. Cont.-in-part of U.S. Ser. No. 569,044,
abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 5474998	A	19951212	US 1993-971974	19930216
WO 9203421	A2	19920305	WO 1991-US5334	19910801
WO 9203421	A3	19921029		
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
PRIORITY APPLN. INFO.:			US 1990-569044	B2 19900817
			US 1990-573954	B2 19900827
			US 1990-595151	B2 19901009
			WO 1991-US5334	W 19910801
OTHER SOURCE(S):			MARPAT 124:202246	
GI				

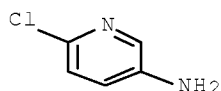


AB Arthropodicidal pyrazoline, pyrazolidine and hydrazine compds. are claimed, including all their geometric and stereoisomers, agriculturally suitable salts thereof and compns. containing them, and a method for controlling arthropods employing said compds. which are QC(:X)NYG and QCX1:NG wherein Q = e.g., I with A = e.g., CH₂, CH₂CH₂, O, OCH₂; R₂ = e.g., H, Cl-6 alkyl, Cl-6 haloalkyl; R₃ = e.g., H, CN, epoxyalkyl; n = 1-3; G = e.g., (un)substituted pyridyl, pyrimidinyl, Ph; X = e.g., O, S; X₁ = e.g., Cl, Br; Y = e.g., H, Cl-6 alkyl, benzyl. Thus, e.g., epoxidn. of 7-chloro-3a-ethenyl-2,3,3a,4-tetrahydro-N-[4-(trifluoromethyl)phenyl][1]benzopyrano[4,3-c]pyrazole-2-carboxamide afforded two oxiranyl diastereomers II which exhibited mortality levels of 80% or higher against, e.g., tobacco budworm, aster leafhopper, and boll weevil at 0.55 kg/ha.

IT 5350-93-6, 5-Amino-2-chloropyridine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (arthropodicidal pyrazolines, pyrazolidines and hydrazines)

RN 5350-93-6 ZCAPLUS

CN 3-Pyridinamine, 6-chloro- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L64 ANSWER 4 OF 4 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1992:426559 ZCAPLUS Full-text
 DOCUMENT NUMBER: 117:26559
 ORIGINAL REFERENCE NO.: 117:4803a,4806a
 TITLE: Preparation of arthropodicidal benzopyranopyrazolecarboxamides, -carboxylates, and related compounds
 INVENTOR(S): Harrison, Charles Richard; Lett, Renee Marie; McCann, Stephen Frederick; Shapiro, Rafael; Stevenson, Thomas Martin
 PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA
 SOURCE: PCT Int. Appl., 291 pp.

10/583635

CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9203421	A2	19920305	WO 1991-US5334	19910801
WO 9203421	A3	19921029		
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
EP 543930	A1	19930602	EP 1991-916421	19910801
R: DE, ES, FR, GB, IT				
JP 06500333	T	19940113	JP 1991-515611	19910801
US 5474998	A	19951212	US 1993-971974	19930216
PRIORITY APPLN. INFO.:			US 1990-569044	A2 19900817
			US 1990-573954	A2 19900827
			US 1990-595151	A2 19901009
			WO 1991-US5334	W 19910801
OTHER SOURCE(S):	MARPAT 117:26559			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

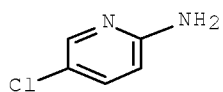
AB The title compds. QC(:X)N(Y)G and QC(X1)(:NG) [Q = Q1-Q5; A = CH2, CH2CH2, O, S, NR5, etc.; G = (un)substituted pyridinyl, -pyrimidinyl, -phenyl(amino), etc.; X = O, S, NX2; X1 = Cl, Br, OR6, etc.; X2 = HO, cyano, SO2Ph, R6, etc.; Y, Y1 = H, C1-6 alkyl(thio), C2-6 alkoxycarbonyl, PhCH2, CHO, etc.; Z (un)substituted = (CH2)q, CH2OCH2, etc.; V = O, S, NR5, R2 = H, C1-6 (halo)alkyl, C2-6 (halo)alkenyl, cyano, NO2, etc.; R3 = Ra, Rb, J; Ra = H, C1-6 (halo)alkyl; Rb = cyano, azido, etc.; J = (un)saturated 5- or 6-membered (un)substituted heteroring; R4 = H, C1-6 (halo)alkyl, (un)substituted Ph, etc.; R5 = H, C1-6 (halo)alkyl, S(O)R15, etc.; R6 = C1-3 alkyl, (un)substituted benzyl, etc.; R15 = H, C1-6 (halo)alkyl, (un)substituted Ph, etc.; R18 = H, C1-4 (halo)alkyl, C4-7 alkylcycloalkyl, etc.; R19 = H, C1-3 alkyl, CO2R15, etc.; R32 = H, Me, CO2Me; n = 1-3, q = 2-4; with a proviso] were prepared as pesticides. Condensation of 2-acetyl-5-chlorothiophene with MeMgBr in Et2O followed by dehydration of the intermediate carbinol gave 2-chloro-5-(1-methylethenyl)thiophene. This was chlorinated by NBS/(PhSe)2 in CH2Cl2/pyridine, the mixture of the resulting vinylic and allylic chlorides in DMF was etherified with 4,2-CF3(HO)C6H3CHO, and the product chromatographed to give 2-[[2-(5-chloro-2-thienyl)-2-propenyl]oxy]-4-(trifluoromethyl)benzaldehyde. The aldehyde was condensed with (EtO)2P(O)NHNH2 in EtOH, the hydrazide cyclized by NBS/Et3N in CH2Cl2, the resulting (benzopyranopyrazolyl)phosphonate was dephosphorylated by Me3SiCl in EtOH, and condensed with 4-CF3C6H4NCO in CH2Cl2 to give title compound (I). I at .apprx.0.55 kg/ha killed ≥80% 3d-instar larvae of Spodoptera frugiperda, Heliothis virescens, and Diabrotica undecimpunctata.

IT 1072-98-6, 2-Amino-5-chloropyridine 5350-93-6,
 5-Amino-2-chloropyridine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation of, in preparation of pesticides)

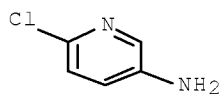
RN 1072-98-6 ZCAPLUS

CN 2-Pyridinamine, 5-chloro- (CA INDEX NAME)

10/583635



RN 5350-93-6 ZCAPLUS
CN 3-Pyridinamine, 6-chloro- (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
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STRUCTURE FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8
DICTIONARY FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> file zcaplus

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FILE COVERS 1907 - 6 Mar 2009 VOL 150 ISS 11
FILE LAST UPDATED: 5 Mar 2009 (20090305/ED)

ZCAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'ZCAPLUS' FILE

=> d stat que L13

10/583635

L2 9 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (1317-38-0/BI OR
2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9

L4 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L2 AND NC5/ES

L5 5 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L4 NOT L3

L8 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9/CRN

L9 572 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (462-08-8/CRN OR
6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR
N)

L10 2 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L8 OR L3

L11 575 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L9 OR L5

L12 23 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L10 (L) PREP/RL

L13 5 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L11 AND L12

=> d stat que L21

L2 9 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (1317-38-0/BI OR
2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9

L4 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L2 AND NC5/ES

L5 5 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L4 NOT L3

L8 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9/CRN

L9 572 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (462-08-8/CRN OR
6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR
N)

L10 2 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L8 OR L3

L11 575 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L9 OR L5

L12 23 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L10 (L) PREP/RL

L13 5 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L11 AND L12

L14 544228 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON CU/ELS

L15 TRANSFER PLU=ON L13 1- RN : 99 TERMS

L16 99 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L15

L17 5 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L14 AND L16

L18 14680 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON ?NITRIT?/CNS

L19 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L16 AND L18

L21 2 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L13 AND (L17 OR L19)

=> d stat que L22

L2 9 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (1317-38-0/BI OR
2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9

L4 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L2 AND NC5/ES

L5 5 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L4 NOT L3

L8 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9/CRN

L9 572 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (462-08-8/CRN OR
6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR
N)

L10 2 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L8 OR L3

L11 575 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L9 OR L5

L12 23 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L10 (L) PREP/RL

L13 5 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L11 AND L12

L22 3 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L13 AND (CU/BI OR
COPPER?/BI OR CUPR?/BI)

=> d stat que L36

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L2          9 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR
              2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
              OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3          1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9
L4          6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
L5          5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3
L14         544228 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  CU/ELS
L23         16 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  C5H3CL2N/MF
L26         109 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1001003-85-5/CRN OR
              1001003-86-6/CRN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR
              1001003-91-3/CRN OR 1001003-97-9/CRN OR 16110-09-1/CRN OR
              2402-77-9/CRN OR 2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/C
              RN OR 26452-80-2/CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR
              851516-88-6/CRN OR 98136-41-5/CRN)

L27         125 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L23 OR L26
L28         571 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (C5H5CLN2.CLH/MF OR
              C5H5CLN2/MF OR C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)

L29         151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L28 AND NC5/ES
L30         151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L5 OR L29
L31         209 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 (L) PREP/RL
L32         23 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L30 AND L31
L33         TRANSFER PLU=ON  L32 1- RN :      7677 TERMS
L34         7677 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L33
L35         6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L34 AND L14
L36         3 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L32 AND L35

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=> d stat que L39

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L2          9 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1317-38-0/BI OR
              2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
              OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3          1 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  2402-77-9
L4          6 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L2 AND NC5/ES
L5          5 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L4 NOT  L3
L23         16 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  C5H3CL2N/MF
L26         109 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (1001003-85-5/CRN OR
              1001003-86-6/CRN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR
              1001003-91-3/CRN OR 1001003-97-9/CRN OR 16110-09-1/CRN OR
              2402-77-9/CRN OR 2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/C
              RN OR 26452-80-2/CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR
              851516-88-6/CRN OR 98136-41-5/CRN)

L27         125 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L23 OR L26
L28         571 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  (C5H5CLN2.CLH/MF OR
              C5H5CLN2/MF OR C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)

L29         151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L28 AND NC5/ES
L30         151 SEA FILE=REGISTRY SPE=ON  ABB=ON  PLU=ON  L5 OR L29
L31         209 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L27 (L) PREP/RL
L32         23 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L30 AND L31
L37         7 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L32 AND (CU/BI OR
              COPPER?/BI OR CUPR?/BI)

L38         9735 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L30 (L) RACT/RL
L39         3 SEA FILE=ZCAPLUS SPE=ON  ABB=ON  PLU=ON  L38 AND L37

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=> d stat que L51

10/583635

L2 9 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (1317-38-0/BI OR
2402-77-9/BI OR 462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI
OR 7447-39-4/BI OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3 1 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 2402-77-9

L4 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L2 AND NC5/ES

L5 5 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L4 NOT L3

L9 572 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (462-08-8/CRN OR
6298-19-7/CRN OR 73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CR
N)

L11 575 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L9 OR L5

L23 16 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON C5H3CL2N/MF

L26 109 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (1001003-85-5/CRN OR
1001003-86-6/CRN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR
1001003-91-3/CRN OR 1001003-97-9/CRN OR 16110-09-1/CRN OR
2402-77-9/CRN OR 2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/C
RN OR 26452-80-2/CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR
851516-88-6/CRN OR 98136-41-5/CRN)

L27 125 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L23 OR L26

L28 571 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON (C5H5CLN2.CLH/MF OR
C5H5CLN2/MF OR C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)

L29 151 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L28 AND NC5/ES

L31 209 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L27 (L) PREP/RL

L42 721 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L11 OR L29

L43 721 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L42 AND NC5/ES

L50 9763 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L43 (L) RACT/RL

L51 5 SEA FILE=ZCAPLUS SPE=ON ABB=ON PLU=ON L50 AND L31

=> s L13 or L21 or L22 or L36 or L51 or L39
L65 8 L13 OR L21 OR L22 OR L36 OR L51 OR L39

=> file casreact
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FILE CONTENT:1840 - 2 Mar 2009 VOL 150 ISS 10

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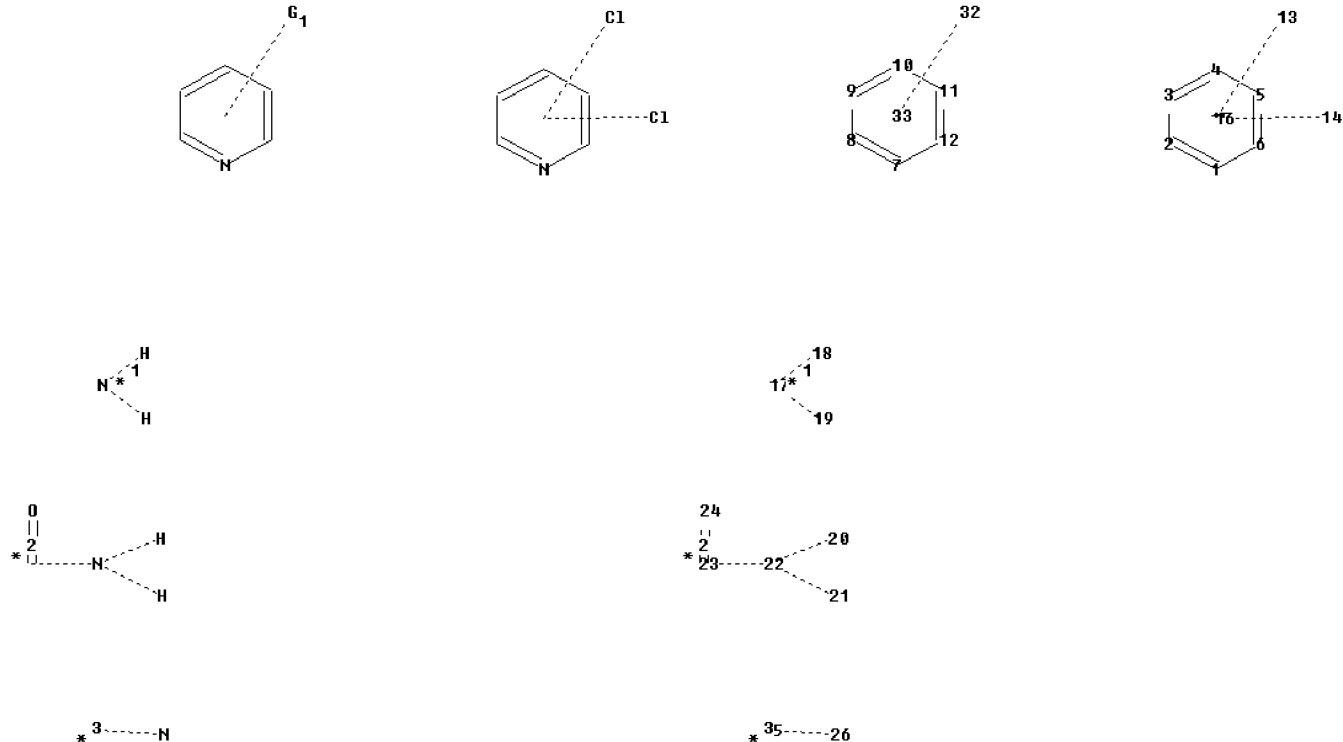
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* *****

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10/583635

This file contains CAS Registry Numbers for easy and accurate substance identification.

Uploading L52.str



```

chain nodes :
13 14 17 18 19 20 21 22 23 24 25 26 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

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G1:[*1],[*2],[*3]

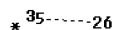
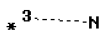
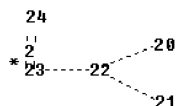
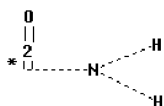
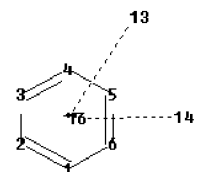
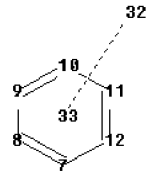
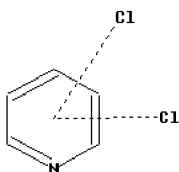
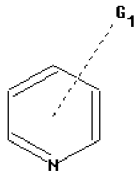
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Connectivity :
25:2 E exact RC ring/chain 26:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 32:CLASS 33:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 7
node mappings:
1:7

```

10/583635

Uploading L58.str



```
chain nodes :
13 14 17 18 19 20 21 22 23 24 25 26 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
```

G1:[*1],[*2],[*3]

```
Connectivity :
25:2 E exact RC ring/chain 26:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 32:CLASS 33:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 7
reaction site bonds:
13-15:CC
```


10/583635

node mappings:

1:7

=> => d stat que L67

L52 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L54 30743 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON CU/ELS AND CASREACT/L
C

L55 51052 SEA FILE=CASREACT SPE=ON ABB=ON PLU=ON L54

L57 12 SEA FILE=CASREACT SUB=L55 SSS FUL L52 (77 REACTIONS)

L58 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

L60 5 SEA FILE=CASREACT SUB=L57 SSS FUL L58 (12 REACTIONS)

L67 5 SEA FILE=CASREACT SPE=ON ABB=ON PLU=ON L55 (L) L60

=> dup rem L67 L65

FILE 'CASREACT' ENTERED AT 12:49:21 ON 06 MAR 2009

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PROCESSING COMPLETED FOR L67

PROCESSING COMPLETED FOR L65

L68 11 DUP REM L67 L65 (2 DUPLICATES REMOVED)

ANSWERS '1-5' FROM FILE CASREACT

ANSWERS '6-11' FROM FILE ZCAPLUS

=> d ibib abs hit L68 1-5; d ibib abs hitind hitstr L68 6-11

L68 ANSWER 1 OF 11 CASREACT COPYRIGHT 2009 ACS on STN DUPLICATE 1

ACCESSION NUMBER: 145:188734 CASREACT Full-text

TITLE: Preparation method for 2,3-dichloropyridine from
3-aminopyridine

INVENTOR(S): Zhao, Taolin; Liu, Aiguo

PATENT ASSIGNEE(S): Nanjing Guangtong Pharmaceutical and Chemical Co.,
Ltd., Peop. Rep. China

SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 7 pp.
CODEN: CNXXEV

DOCUMENT TYPE: Patent

LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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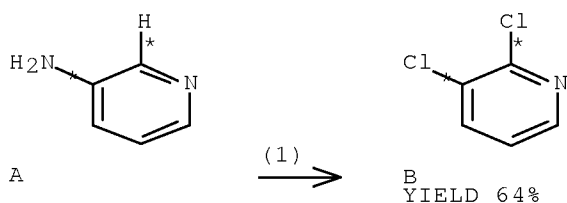
10/583635

CN 1807414 A 20060726 CN 2006-10038159 20060206
 CN 100357272 C 20071226

PRIORITY APPLN. INFO.: CN 2006-10038159 20060206

AB The title preparation method includes 2-chlorination of 3-aminopyridine with hydrogen peroxide (content <20%) at a molar ratio of 1:1 in concentrated hydrochloric acid (content ≤31%) at 6-8 °C for 1-2 h; diazotizing with 30% sodium nitrite solution (at equal mole to the 3-aminopyridine) at <0 °C for 0.5-1 h; 3-chlorination with mixture of cuprous chloride (0.15 M times of 3-aminopyridine) and concentrated hydrochloric acid (2 M times of 3-aminopyridine) at <0 °C for >30 min; extracting with dichloromethane at room temperature; and vacuum distilling solvent out to obtain 2,3-dichloropyridine.

RX(1) OF 1 A ==> B



RX(1) RCT A 462-08-8

STAGE(1)

RGT C 7647-01-0 HCl, D 7722-84-1 H2O2
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) room temperature -> 30 deg C
 SUBSTAGE(2) 30 deg C -> 4 deg C
 SUBSTAGE(3) 52 minutes, 6 - 8 deg C
 SUBSTAGE(4) 1 hour, 6 - 8 deg C
 SUBSTAGE(5) 8 deg C -> -8 deg C

STAGE(2)

RGT E 7632-00-0 NaNO2
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 25 minutes, -8 - -5 deg C
 SUBSTAGE(2) 30 minutes, -8 - -5 deg C
 SUBSTAGE(3) -5 deg C -> -10 deg C

STAGE(3)

RGT C 7647-01-0 HCl
 CAT 7758-89-6 CuCl
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) 63 minutes, -10 - -5 deg C
 SUBSTAGE(2) 1 hour, -5 - 0 deg C
 SUBSTAGE(3) 0 deg C -> room temperature

PRO B 2402-77-9

NTE regioselective, optimization study, optimized on the reaction temperature and time

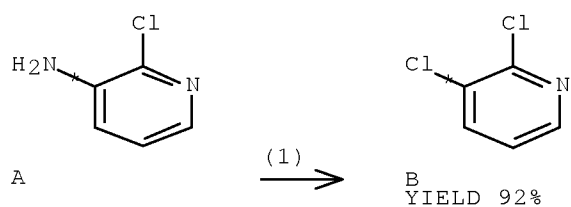
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WO 2005070888		A2	20050804	WO 2005-US2462		20050121
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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2005206576		A1	20050804	AU 2005-206576		20050121
CA 2553850		A1	20050804	CA 2005-2553850		20050121
EP 1706381		A2	20061004	EP 2005-712075		20050121
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS, YU					
CN 1910152		A	20070207	CN 2005-80002691		20050121
BR 2005006502		A	20070227	BR 2005-6502		20050121
JP 2007523065		T	20070816	JP 2006-551437		20050121
US 20070161797		A1	20070712	US 2006-583635		20060620
IN 2006DN03640		A	20070824	IN 2006-DN3640		20060623
MX 2006008208		A	20060831	MX 2006-8208		20060719
KR 2006130618		A	20061219	KR 2006-714736		20060721
PRIORITY APPLN. INFO.:				US 2004-539068P		20040123
				WO 2005-US2462		20050121

AB A method for preparing 2,3-dichloropyridine is disclosed in which 3-amino-2-chloropyridine is contacted with an alkali metal nitrite in the presence of aqueous hydrochloric acid to form a diazonium salt; and the diazonium salt is subsequently decomposed in the presence of copper catalyst wherein at least about 50% of the copper is the copper(II) oxidation state.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

19

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RX(1) RCT A ~~6298-19-7~~

STAGE(1)

RGT C 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature -> -8 deg C

STAGE(2)

RGT D 7632-00-0 NaNO2

SOL 7732-18-5 Water

CON 30 minutes, -7 - -3 deg C

STAGE(3)

RGT C 7647-01-0 HCl

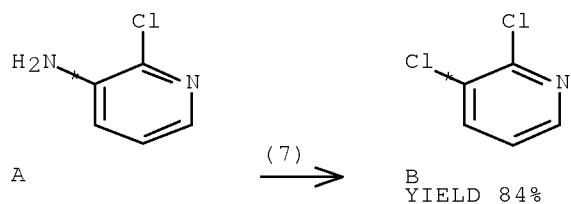
CAT ~~1317-38-0~~ CuO

SOL 109-69-3 BuCl, 7732-18-5 Water

CON 55 - 62 deg C

PRO B ~~2402-77-9~~

RX(7) OF 11 A ==> B



RX(7) RCT A ~~6298-19-7~~

STAGE(1)

RGT D 7632-00-0 NaNO2

SOL 7732-18-5 Water

CON 30 minutes, -5 - 0 deg C

STAGE(2)

RGT C 7647-01-0 HCl

CAT ~~7447-39-4~~ CuCl2

SOL 109-69-3 BuCl, 7732-18-5 Water

CON SUBSTAGE(1) 1 hour, 60 deg C

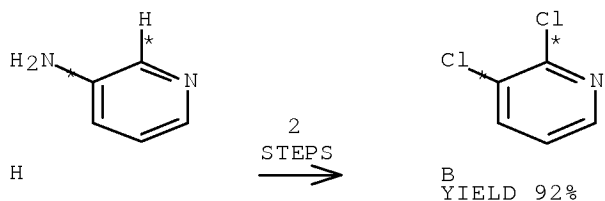
10/583635

SUBSTAGE(2) 30 minutes, 60 deg C

PRO B 2402--77--9

RX(8) OF 11 COMPOSED OF RX(2), RX(1)

RX(8) H ==> B



RX(2) RCT H 462--08--8

STAGE(1)

RGT C 7647-01-0 HCl

SOL 7732-18-5 Water

CON 30 - 35 deg C

STAGE(2)

RGT I 7722-84-1 H2O2

SOL 7732-18-5 Water

CON SUBSTAGE(1) 20 minutes, 10 - 12 deg C

SUBSTAGE(2) 2 hours, 10 deg C

SUBSTAGE(3) 2 hours, 10 deg C -> 19 deg C

SUBSTAGE(4) 4 hours, 19 deg C

STAGE(3)

RGT J 7757-83-7 Na2SO3

SOL 7732-18-5 Water

CON 10 deg C

STAGE(4)

RGT K 1310-73-2 NaOH

SOL 7732-18-5 Water, 108-88-3 PhMe

CON 25 - 35 deg C

PRO A 6298-19-7

RX(1) RCT A 6298-19-7

STAGE(1)

RGT C 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature -> -8 deg C

STAGE(2)

RGT D 7632-00-0 NaNO2

SOL 7732-18-5 Water

CON 30 minutes, -7 - -3 deg C

10/583635

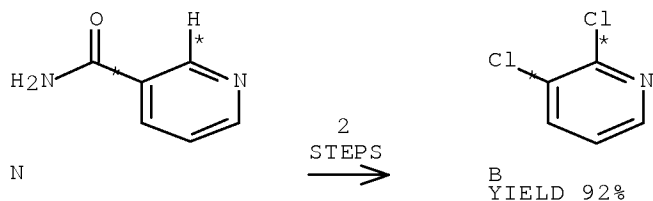
STAGE(3)

RGT C 7647-01-0 HCl
CAT 1317-38-0 CuO
SOL 109-69-3 BuCl, 7732-18-5 Water
CON 55 - 62 deg C

PRO B 2402-77-9

RX(9) OF 11 COMPOSED OF RX(4), RX(1)

RX(9) N ==> B



RX(4) RCT N 98-92-0

STAGE(1)

RGT O 7681-52-9 NaOCl
SOL 7732-18-5 Water
CON 30 minutes, 0 - 5 deg C

STAGE(2)

RGT K 1310-73-2 NaOH
SOL 7732-18-5 Water
CON 30 minutes, 0 - 5 deg C

STAGE(3)

SOL 7732-18-5 Water
CON SUBSTAGE(1) 40 minutes, 75 - 81 deg C
SUBSTAGE(2) 15 minutes, 80 deg C

STAGE(4)

RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON 40 - 50 deg C

STAGE(5)

RGT I 7722-84-1 H2O2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 1.5 hours, 10 deg C
SUBSTAGE(2) 2 hours, room temperature
SUBSTAGE(3) 30 minutes, room temperature

STAGE(6)

RGT K 1310-73-2 NaOH, J 7757-83-7 Na2SO3
SOL 7732-18-5 Water, 108-88-3 PhMe
CON 15 - 25 deg C

PRO A 6298-19-7

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RX(1) RCT A 6298-19-7

STAGE(1)

RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature -> -8 deg C

STAGE(2)

RGT D 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 30 minutes, -7 - -3 deg C

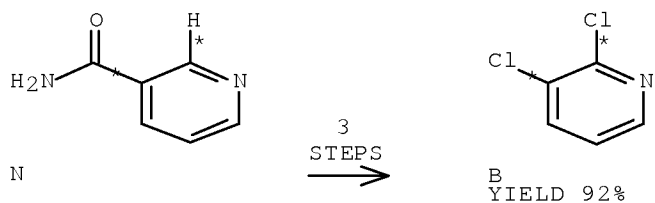
STAGE(3)

RGT C 7647-01-0 HCl
CAT ~~1317-38-0~~ CuO
SOL 109-69-3 BuCl, 7732-18-5 Water
CON 55 - 62 deg C

PRO B ~~2402-77-9~~

RX(11) OF 11 COMPOSED OF RX(5), RX(2), RX(1)

RX(11) N ==> B



RX(5) RCT N ~~98-92-0~~

STAGE(1)

RGT O 7681-52-9 NaOCl
SOL 7732-18-5 Water
CON SUBSTAGE(1) 30 minutes, 0 deg C
SUBSTAGE(2) 15 minutes, 0 deg C

STAGE(2)

RGT K 1310-73-2 NaOH
SOL 7732-18-5 Water
CON 30 minutes, 0 - 5 deg C

STAGE(3)

SOL 7732-18-5 Water
CON SUBSTAGE(1) 30 minutes, 90 deg C
SUBSTAGE(2) 1 hour, 90 deg C

STAGE(4)

RGT C 7647-01-0 HCl
SOL 7732-18-5 Water

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CON SUBSTAGE(1) 45 minutes, 40 deg C
SUBSTAGE(2) overnight, room temperature

PRO H 462-08-8

RX(2) RCT H 462-08-8

STAGE(1)

RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON 30 - 35 deg C

STAGE(2)

RGT I 7722-84-1 H2O2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 20 minutes, 10 - 12 deg C
SUBSTAGE(2) 2 hours, 10 deg C
SUBSTAGE(3) 2 hours, 10 deg C -> 19 deg C
SUBSTAGE(4) 4 hours, 19 deg C

STAGE(3)

RGT J 7757-83-7 Na2SO3
SOL 7732-18-5 Water
CON 10 deg C

STAGE(4)

RGT K 1310-73-2 NaOH
SOL 7732-18-5 Water, 108-88-3 PhMe
CON 25 - 35 deg C

PRO A 6298-19-7

RX(1) RCT A 6298-19-7

STAGE(1)

RGT C 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature -> -8 deg C

STAGE(2)

RGT D 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON 30 minutes, -7 - -3 deg C

STAGE(3)

RGT C 7647-01-0 HCl
CAT ~~1317-38-0~~ CuO
SOL 109-69-3 BuCl, 7732-18-5 Water
CON 55 - 62 deg C

PRO B ~~2402-77-9~~

L68 ANSWER 3 OF 11 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 142:447087 CASREACT Full-text

TITLE: Removal of fluorine from and introduction of fluorine
into polyhalopyridines: an exercise in nucleophilic
hetarenic substitution

AUTHOR(S): Bobbio, Carla; Rausis, Thierry; Schlosser, Manfred

CORPORATE SOURCE: Institute of Chemical Sciences and Engineering, Ecole

10/583635

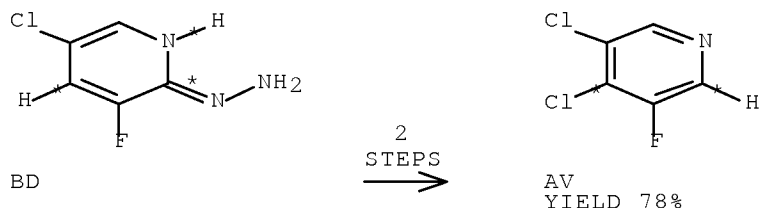
SOURCE: Polytechnique Federale, Lausanne, 1015, Switz.
Chemistry--A European Journal (2005), 11(6), 1903-1910
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Starting from six industrially available fluorinated pyridines, an expedient access to all three tetrafluoropyridines, all six trifluoropyridines, and the five non-com. difluoropyridines was developed. The methods employed for the selective removal of fluorine from polyfluoropyridines were the reduction by metals or complex hydrides and the site-selective replacement by hydrazine followed by dehydrogenation-dediazotation or dehydrochlorination-dediazotation. To introduce an extra fluorine atom, a suitable precursor was metalated and chlorinated before being subjected to a chlorine/fluorine displacement process.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(62) OF 136 COMPOSED OF RX(24), RX(23)

RX(62) BD ==> AV



RX(24) RCT BD 248255-70-1
RGT T 7758-98-7 CuSO4
PRO BC 514797-99-0
SOL 7732-18-5 Water
CON 2 hours, reflux

RX(23) RCT BC 514797-99-0

STAGE(1)

RGT AP 109-72-8 BuLi
SOL 109-99-9 THF, 110-54-3 Hexane
CON 2 hours, -75 deg C

STAGE(2)

RGT AW 76-13-1 Freon 113
CON 1 hour, -75 deg C

PRO AV 851179-02-7

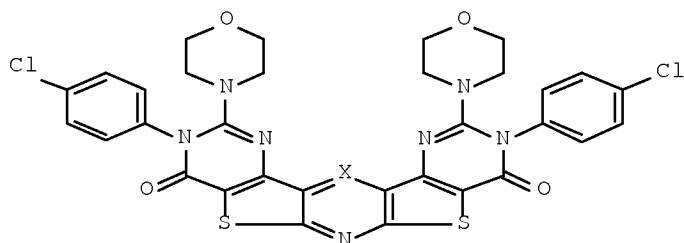
L68 ANSWER 4 OF 11 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 140:163819 CASREACT Full-text

TITLE: Synthesis of pyrido and
pyrazinodithienodiprimidine-4,8(3H,9H)-dione
derivatives by the aza-Wittig methodology

10/583635

AUTHOR(S): Vilarelle, David Vazquez; Veira, Carlos Peinador; Quintela Lopez, Jose M.
 CORPORATE SOURCE: Facultad de Ciencias, Departamento de Quimica Fundamental, Universidad de La Coruna, La Coruna, E-15071, Spain
 SOURCE: Tetrahedron (2004), 60(2), 275-283
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

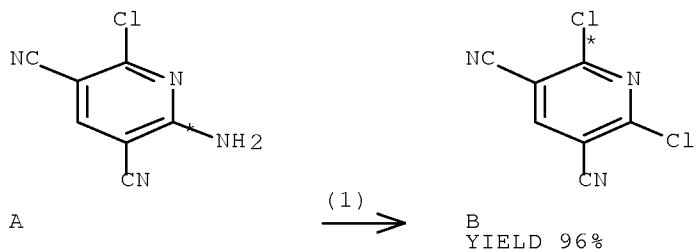


I

AB A one-pot synthesis of the hitherto unreported pyrido[5'',6'':4,5;3''2'':4',5']dithieno[3,2-d:3',2'-d']dipyrimidine-4,8(3H,9H)-diones, e.g. I (X = CH), and pyrazino[5'',6'':4,5;3''2'':4',5']dithieno[3,2-d:3',2'-d']dipyrimidine-4,8(3H,9H)-diones, e.g. I (X = N) pentaheterocyclic systems, based on the tandem aza-Wittig heterocumulene-mediated annulation strategy, is described.

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 157 A ==> B...



RX(1) RCT A 51768-01-5

STAGE(1)

RGT C 7447-39-4 CuCl2, D 110-46-3 Isoamyl nitrite
 SOL 75-05-8 MeCN

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CON 5 hours, 65 deg C

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

CON room temperature, acidify

PRO B 151229-84-4

L68 ANSWER 5 OF 11 CASREACT COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 137:353202 CASREACT Full-text

TITLE: Synthesis, Nicotinic Acetylcholine Receptor Binding, and Antinociceptive Properties of 2-exo-2-(2',3'-Disubstituted 5'-pyridinyl)-7-azabicyclo[2.2.1]heptanes: Epibatidine Analogues

AUTHOR(S): Carroll, F. Ivy; Lee, Jeffrey R.; Navarro, Hernan A.; Ma, Wei; Brieady, Lawrence E.; Abraham, Philip; Damaj, M. I.; Martin, Billy R.

CORPORATE SOURCE: Chemistry and Life Sciences, Research Triangle Institute, Research Triangle Park, NC, 27709, USA

SOURCE: Journal of Medicinal Chemistry (2002), 45(21), 4755-4761

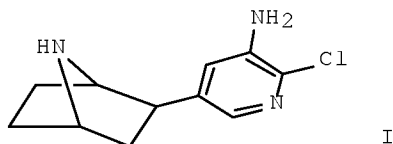
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



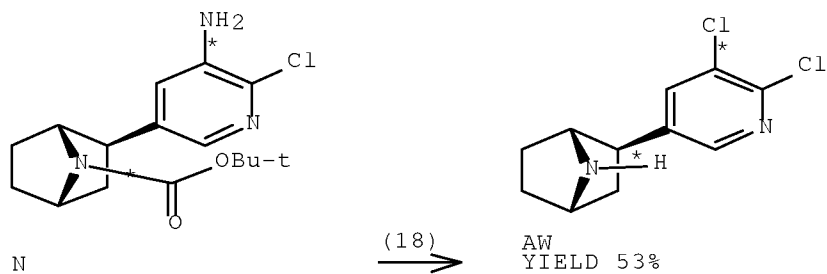
AB A number of 2',3'-disubstituted epibatidine analogs were synthesized and evaluated in vitro for potency at nicotinic acetylcholine receptors (nAChRs) and in vivo for antinociception activity in the tail-flick and hot-plate models of acute pain and for their ability to affect core body temperature. Compds. that possessed electron-withdrawing groups (F, Cl, Br, and I) in both the 2'- and the 3'-positions showed affinities at the nAChR similar to epibatidine. However, in vivo efficacy did not correlate with affinity. 2-Exo-(3'-Amino-2'-chloro-5'-pyridinyl)-7- azabicyclo[2.2.1]heptane (I), an epibatidine analog possessing an electron-releasing amino group in the 3'-position, produced the highest affinity. Compound I was also the most selective epibatidine analog with a K_i of 0.001 nM at $\alpha\beta$ nAChRs, which is 26 times greater than that of epibatidine, and a $\alpha\beta/\alpha\gamma$ K_i ratio of 14 000, twice that of epibatidine. In vivo testing revealed that this compound potently inhibited nicotine-induced antinociception with AD₅₀ values below 1 μ g/kg. Surprisingly, this same compound was also an agonist at higher doses (ED₅₀ .apprx.20 μ g/kg). Thus, the addition of the 3'-amino group to epibatidine

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confers potent antagonist activity to the compound with little effect on agonist activity. 2,3-Disubstituted epibatidine analogs possessing a 2'-amino group combined with a 3'-bromo or 3'-iodo group showed in vitro and in vivo nAChR properties similar to nicotine.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

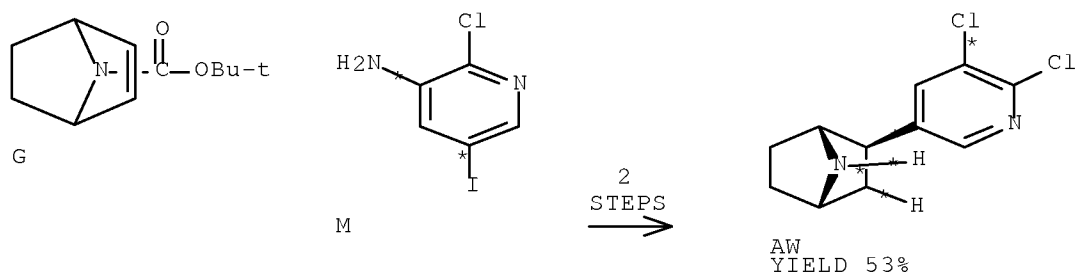
RX(18) OF 95 ...N ==> AW



RX(18) RCT N 426461-98-5
RGT X 7647-01-0 HCl, D 7632-00-0 NaNO2, Y 7758-89-6 CuCl
PRO AW 426460-53-9
SOL 7732-18-5 Water

RX(32) OF 95 COMPOSED OF RX(3), RX(18)

RX(32) G + M ==> AW



RX(3) RCT G 192118-47-1, M 426463-09-4

STAGE(1)

RGT I 590-29-4 HCO2K
CAT 3375-31-3 Pd(OAc)2, 1112-67-0 Bu4NC1
SOL 68-12-2 DMF

STAGE(2)

RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO N 426461-98-5

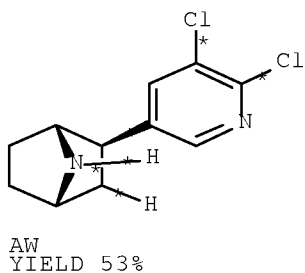
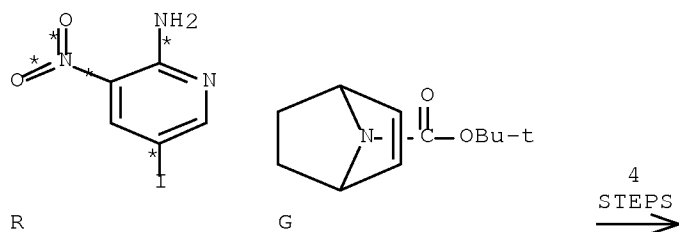
10/583635

NTE stereoselective

RX(18) RCT N 426461-98-5
RGT X 7647-01-0 HCl, D 7632-00-0 NaNO2, Y 7758-89-6 CuCl
PRO AW 426460-53-9
SOL 7732-18-5 Water

RX(69) OF 95 COMPOSED OF RX(6), RX(8), RX(3), RX(18)

RX(69) R + G ==> AW



RX(6) RCT R 25391-57-5

STAGE(1)

RGT X 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)

RGT D 7632-00-0 NaNO2, Y 7758-89-6 CuCl

STAGE(3)

RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO W 426463-05-0

RX(8) RCT W 426463-05-0
RGT X 7647-01-0 HCl, AB 7439-89-6 Fe
PRO M 426463-09-4
SOL 64-17-5 EtOH, 7732-18-5 Water

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RX(3) RCT G 192118-47-1, M 426463-09-4

STAGE(1)

RGT I 590-29-4 HCO2K

CAT 3375-31-3 Pd(OAc)2, 1112-67-0 Bu4NC1

SOL 68-12-2 DMF

STAGE(2)

RGT E 1336-21-6 NH4OH

SOL 7732-18-5 Water

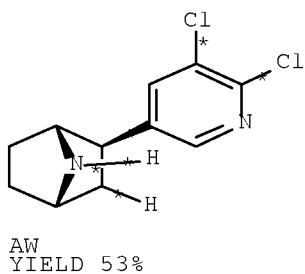
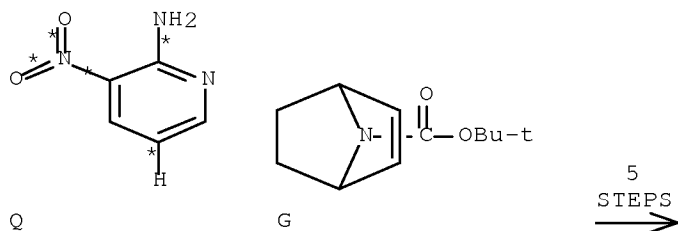
PRO N 426461-98-5

NTE stereoselective

RX(18) RCT N 426461-98-5
RGT X 7647-01-0 HCl, D 7632-00-0 NaNO2, Y 7758-89-6 CuCl
PRO AW 426460-53-9
SOL 7732-18-5 Water

RX(82) OF 95 COMPOSED OF RX(5), RX(6), RX(8), RX(3), RX(18)

RX(82) Q + G ==> AW



RX(5) RCT Q 4214-75-9

STAGE(1)

RGT S 7553-56-2 I2

CAT 10450-60-9 H5IO6

SOL 64-19-7 AcOH, 7732-18-5 Water

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STAGE(2)
RGT T 7772-98-7 Na2S2O3
SOL 7732-18-5 Water

PRO R 25391-57-5

RX(6) RCT R 25391-57-5

STAGE(1)
RGT X 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT D 7632-00-0 NaNO2, Y ~~7758-89-6~~ CuCl

STAGE(3)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO W 426463-05-0

RX(8) RCT W 426463-05-0
RGT X 7647-01-0 HCl, AB 7439-89-6 Fe
PRO M 426463-09-4
SOL 64-17-5 EtOH, 7732-18-5 Water

RX(3) RCT G 192118-47-1, M 426463-09-4

STAGE(1)
RGT I 590-29-4 HCO2K
CAT 3375-31-3 Pd(OAc)2, 1112-67-0 Bu4NCl
SOL 68-12-2 DMF

STAGE(2)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO N 426461-98-5
NTE stereoselective

RX(18) RCT N 426461-98-5
RGT X 7647-01-0 HCl, D 7632-00-0 NaNO2, Y ~~7758-89-6~~ CuCl
PRO AW ~~426460-53-9~~
SOL 7732-18-5 Water

L68 ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:1369724 ZCAPLUS Full-text
DOCUMENT NUMBER: 150:19997
TITLE: Method for preparing 2,3-dichloropyridine
INVENTOR(S): Liu, Xiaomin
PATENT ASSIGNEE(S): Hebei Yanuo Chemical Industry Co., Ltd., Peop. Rep.
China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 10pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101302190	A	20081112	CN 2008-10055291	20080630
PRIORITY APPLN. INFO.:			CN 2008-10055291	20080630

AB The title method comprises the steps of: dissolving 3-aminopyridine into concentrated HCl acid to obtain a HCl acid solution of 3-aminopyridine hydrochloride, performing chlorination onto 3-aminopyridine with chlorinating agents with Fe²⁺ or Fe³⁺ as catalyst to obtain a system containing mainly 2-chloro-3-aminopyridine, performing diazotization/chlorination with sodium nitrite with Cu⁺ and/or Cu²⁺ as catalyst to obtain 2,3-dichloropyridine, adjusting the pH to above 7, distilling with water vapor to obtain crude 2,3-dichloropyridine, and recrystg. to obtain refined 2,3-dichloropyridine. The method has high product purity (above 99.2%), and high yield (above 71.4% calculated by 3-aminopyridine).

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

ST dichloropyridine prepn aminopyridine diazotization chlorination catalyst iron copper salt

IT Diazotization catalysts
(copper salt; preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT Chlorination catalysts
(iron/copper salt; preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 1317-38-0, Cupric oxide, uses 1317-39-1, Cuprous oxide, uses 7447-39-4, Cupric chloride, uses 7758-89-6, Cuprous chloride 17599-81-4, Cuprous sulfate
RL: CAT (Catalyst use); USES (Uses)
(diazotization/chlorination catalyst; preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 2402-77-9P, 2,3-Dichloropyridine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 462-08-8, 3-Aminopyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 6298-19-7P, 2-Chloro-3-aminopyridine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 7632-00-0, Sodium nitrite 7647-01-0, Hydrochloric acid, reactions 7722-84-1, Hydrogen peroxide (H₂O₂), reactions 7782-50-5, Chlorine, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)

IT 1317-38-0, Cupric oxide, uses 1317-39-1, Cuprous oxide, uses 7447-39-4, Cupric chloride, uses 7758-89-6, Cuprous chloride 17599-81-4, Cuprous sulfate
RL: CAT (Catalyst use); USES (Uses)
(diazotization/chlorination catalyst; preparation of 2,3-dichloropyridine from 3-aminopyridine)

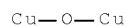
RN 1317-38-0 ZCAPLUS

CN Copper oxide (CuO) (CA INDEX NAME)

10/583635



RN 1317-39-1 ZCAPLUS
CN Copper oxide (Cu₂O) (CA INDEX NAME)



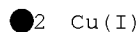
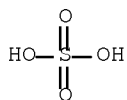
RN 7447-39-4 ZCAPLUS
CN Copper chloride (CuCl₂) (CA INDEX NAME)



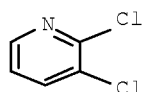
RN 7758-89-6 ZCAPLUS
CN Copper chloride (CuCl) (CA INDEX NAME)



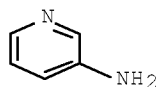
RN 17599-81-4 ZCAPLUS
CN Sulfuric acid, copper(1+) salt (1:2) (CA INDEX NAME)



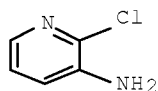
IT 2402-77-9F, 2,3-Dichloropyridine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)
(preparation of 2,3-dichloropyridine from 3-aminopyridine)
RN 2402-77-9 ZCAPLUS
CN Pyridine, 2,3-dichloro- (CA INDEX NAME)



IT 462-08-8, 3-Aminopyridine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of 2,3-dichloropyridine from 3-aminopyridine)
 RN 462-08-8 ZCAPLUS
 CN 3-Pyridinamine (CA INDEX NAME)



IT 6298-19-7P, 2-Chloro-3-aminopyridine
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation of 2,3-dichloropyridine from 3-aminopyridine)
 RN 6298-19-7 ZCAPLUS
 CN 3-Pyridinamine, 2-chloro- (CA INDEX NAME)



IT 7632-00-0, Sodium nitrite
 RL: RGT (Reagent); RACT (Reactant or reagent)
 (preparation of 2,3-dichloropyridine from 3-aminopyridine)
 RN 7632-00-0 ZCAPLUS
 CN Nitrous acid, sodium salt (1:1) (CA INDEX NAME)



L68 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2006:1287458 ZCAPLUS [Full-text](#)
 DOCUMENT NUMBER: 146:183995
 TITLE: Cu(I)-mediated deoxygenation of N-oxides to amines
 AUTHOR(S): Singh, Sunil Kumar; Reddy, M. Srinivasa; Mangle, Mangesh; Ganesh, K. Ravi
 CORPORATE SOURCE: Discovery Chemistry, Discovery Research-Dr. Reddy's Laboratories Ltd., Hyderabad, 500 049, India
 SOURCE: Tetrahedron (2006), Volume Date 2007, 63(1), 126-130
 CODEN: TETRAB; ISSN: 0040-4020
 PUBLISHER: Elsevier Ltd.
 DOCUMENT TYPE: Journal

10/583635

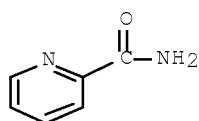
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:183995
AB A mild and highly efficient deoxygenation of variety of N-oxides using an inexpensive CuX (X = I, Cl) or a CuX-Zn or CuX-Al couple is described. Though CuX alone effectively deoxygenates the aliphatic and aromatic N-oxides in aprotic solvents at lower temperature (30-50°C), the CuX-Zn and CuX-Al systems require refluxing the substrates (viz., nitron, azoxybenzene, and heteroarene N-oxides) in ethanol at 50-60°C.
CC 21-2 (General Organic Chemistry)
IT 7429-90-5, Aluminum, uses 7440-66-6, Zinc, uses 7681-65-4, Copper iodide (CuI) 7758-89-6, Copper chloride (CuCl)
RL: CAT (Catalyst use); USES (Uses)
(preparation of amines by Cu(I)-mediated deoxygenation of N-oxides)
IT 91-22-5P, Quinoline, preparation 91-63-4P, 2-Methylquinoline 109-02-4P, 4-Methylmorpholine 109-06-8P, 2-Methylpyridine 109-09-1P, 2-Chloropyridine 110-86-1P, Pyridine, preparation 121-44-8P, Triethylamine, preparation 612-62-4P, 2-Chloroquinoline 702-11-4P 824-21-5P 933-94-8P 1452-77-3P, 2-Pyridinecarboxamide 2402-78-0P, 2,6-Dichloropyridine 2459-07-6P, Methyl 2-pyridinecarboxylate 2632-65-7P 10220-22-1P 16155-03-6P 39769-11-4P 123330-59-6P 329943-64-8P 385380-74-5P 922142-73-2P 922142-74-3P 922142-75-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amines by Cu(I)-mediated deoxygenation of N-oxides)
IT 7681-65-4, Copper iodide (CuI) 7758-89-6, Copper chloride (CuCl)
RL: CAT (Catalyst use); USES (Uses)
(preparation of amines by Cu(I)-mediated deoxygenation of N-oxides)
RN 7681-65-4 ZCAPLUS
CN Copper iodide (CuI) (CA INDEX NAME)

Cu—I

RN 7758-89-6 ZCAPLUS
CN Copper chloride (CuCl) (CA INDEX NAME)

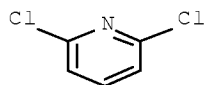
Cl—Cu

IT 1452-77-3P, 2-Pyridinecarboxamide 2402-78-0P, 2,6-Dichloropyridine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of amines by Cu(I)-mediated deoxygenation of N-oxides)
RN 1452-77-3 ZCAPLUS
CN 2-Pyridinecarboxamide (CA INDEX NAME)



10/583635

RN 2402-78-0 ZCAPLUS
CN Pyridine, 2,6-dichloro- (CA INDEX NAME)



REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:270415 ZCAPLUS Full-text
DOCUMENT NUMBER: 134:266210
TITLE: Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine
INVENTOR(S): Yokota, Keiichi; Takeuchi, Seiji
PATENT ASSIGNEE(S): Sumikin Chemical K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 2001106672	A	20010417	JP 1999-284819	19991005
PRIORITY APPLN. INFO.:			JP 1999-284819	19991005

OTHER SOURCE(S): CASREACT 134:266210

AB 2,5-Dichloropyridine (I) is prepared by treatment of 2-amino-5-chloropyridine (II) with NaNO₂ in HCl, and the byproduct, 5-chloro-2-hydroxypyridine (III) is further treated with POCl₃ in the presence of DMF. Thus, II was treated with aqueous NaNO₂ at 40-50° in HCl-MePh, neutralized, and filtered to give crystals containing III. The organic phase of the filtrate was mixed with the crystals, evaporated to dryness, mixed with DMF, and treated with POCl₃ at 100° to give I with 84.5% yield from II.

IC ICM C07D213-61

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

IT 16110-09-1P, 2,5-Dichloropyridine

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine)

IT 1072-98-6, 2-Amino-5-chloropyridine 7632-00-0, Sodium nitrite 7647-01-0, Hydrochloric acid, reactions 10025-87-3, Phosphorus oxychloride

RL: RCT (Reactant); RACT (Reactant or reagent)

(Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine)

IT 16110-09-1P, 2,5-Dichloropyridine

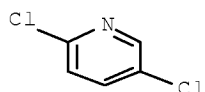
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine)

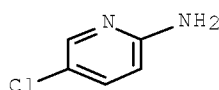
RN 16110-09-1 ZCAPLUS

10/583635

CN Pyridine, 2,5-dichloro- (CA INDEX NAME)



IT 1072-98-6, 2-Amino-5-chloropyridine
RL: RCT (Reactant); RACT (Reactant or reagent)
(Preparation of 2,5-dichloropyridine from 2-amino-5-chloropyridine)
RN 1072-98-6 ZCAPLUS
CN 2-Pyridinamine, 5-chloro- (CA INDEX NAME)



L68 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:314380 ZCAPLUS Full-text

DOCUMENT NUMBER: 125:33445

ORIGINAL REFERENCE NO.: 125:6529a,6532a

TITLE: Substituent effect on the chlorination of
2-alkoxypyridines to give 2-chloropyridines under
Vilsmeier-Haack conditions

AUTHOR(S): Lai, Long-Li; Lin, Pen-Yuan; Wang, Jy-Shih; Hwu, Jih
Ru; Shiao, Min-Jen; Tsay, Shwu-Chen

CORPORATE SOURCE: Inst. Chem., Acad. Sinica, Taipei, 11529, Taiwan

SOURCE: Journal of Chemical Research, Synopses (1996), (4),
194-195

CODEN: JRPSDC; ISSN: 0308-2342

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:33445

AB Various substituted 2-alkoxypyridines were converted into the corresponding 2-chloropyridines in 28-91% yield by use of POCl₃ and DMF. Me, halogen, ester and nitro groups displayed an activating effect and an amino group exhibited a deactivating effect.

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

IT 109-09-1P, 2-Chloropyridine 2402-77-9P, 2,3-Dichloropyridine
2402-78-0P, 2,6-Dichloropyridine 4548-45-2P, 2-Chloro-5-nitropyridine
5140-72-7P, 2-Bromo-6-chloropyridine 5470-18-8P,
2-Chloro-3-nitropyridine 6298-19-7P, 3-Amino-2-chloropyridine
18368-63-3P, 2-Chloro-6-methylpyridine 52200-48-3P,
3-Bromo-2-chloropyridine 73781-91-6P, Methyl
6-chloro-3-pyridinecarboxylate

RL: SPN (Synthetic preparation); PREP (Preparation)

(substituent effect on the chlorination of 2-alkoxypyridines to give
2-chloropyridines under Vilsmeier-Haack conditions)

IT 2402-77-9P, 2,3-Dichloropyridine 6298-19-7P,
3-Amino-2-chloropyridine

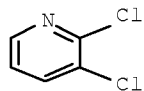
10/583635

RL: SPN (Synthetic preparation); PREP (Preparation)

(substituent effect on the chlorination of 2-alkoxypyridines to give 2-chloropyridines under Vilsmeier-Haack conditions)

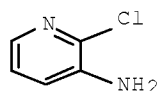
RN 2402-77-9 ZCAPLUS

CN Pyridine, 2,3-dichloro- (CA INDEX NAME)



RN 6298-19-7 ZCAPLUS

CN 3-Pyridinamine, 2-chloro- (CA INDEX NAME)



L68 ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1992:407994 ZCAPLUS Full-text

DOCUMENT NUMBER: 117:7994

ORIGINAL REFERENCE NO.: 117:1619a,1622a

TITLE: Electrophilic aromatic substitution. 39. The mechanism of the carbodesilylation of 4- or 5-substituted 2-(trimethylsilyl)pyridines

AUTHOR(S): Effenberger, Franz; Krebs, Andreas; Willrett, Peter

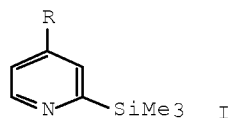
CORPORATE SOURCE: Inst. Org. Chem., Univ. Stuttgart, Stuttgart, W-7000/80, Germany

SOURCE: Chemische Berichte (1992), 125(5), 1131-40
CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

GI

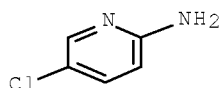


AB An ylide mechanism is proposed for the carbodesilylation of 2-(trimethylsilyl)pyridines with benzaldehyde. In contrast, 3- and 4-(trimethylsilyl)pyridines (e.g., I; R = H, Me, MeO, Cl, CN, PhSO₂, Me₃Si) react only in the presence of a base catalyst via pyridyl anions with electrophiles. The rates of the uncatalyzed carbodesilylation reactions of I

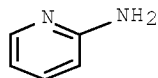
10/583635

with benzaldehyde correlate very well with the resonance parameters of the substituents σ_{R0} , whereas the rates of 5-substituted 2-(trimethylsilyl)pyridines correlate with the inductive substituent parameters σ_I in the Taft equation. This is the first direct determination of the resonance parameters σ_{R0} .

CC 29-6 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22
 IT 695-34-1 1072-98-6 1603-41-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of)
 IT 504-29-0, 2-Aminopyridine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (iodination of)
 IT 5350-93-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation and amination of)
 IT 1453-82-3P, 4-Pyridinecarboxamide 4214-76-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation and oxidation of)
 IT 3510-66-5P 4926-28-7P 22918-01-0P 26452-80-2P 33252-28-7P
 33252-30-1P 40473-01-6P 67743-63-9P 89488-29-9P 139585-48-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and silylation of)
 IT 1072-98-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (bromination of)
 RN 1072-98-6 ZCAPLUS
 CN 2-Pyridinamine, 5-chloro- (CA INDEX NAME)



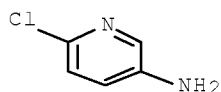
IT 504-29-0, 2-Aminopyridine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (iodination of)
 RN 504-29-0 ZCAPLUS
 CN 2-Pyridinamine (CA INDEX NAME)



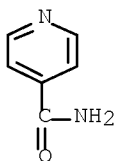
IT 5350-93-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation and amination of)
 RN 5350-93-6 ZCAPLUS

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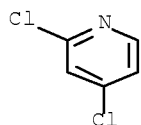
CN 3-Pyridinamine, 6-chloro- (CA INDEX NAME)



IT 1453-82-3P, 4-Pyridinecarboxamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and oxidation of)
RN 1453-82-3 ZCAPLUS
CN 4-Pyridinecarboxamide (CA INDEX NAME)



IT 26452-80-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and silylation of)
RN 26452-80-2 ZCAPLUS
CN Pyridine, 2,4-dichloro- (CA INDEX NAME)



L68 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1989:192171 ZCAPLUS Full-text
DOCUMENT NUMBER: 110:192171
ORIGINAL REFERENCE NO.: 110:31881a,31884a
TITLE: Site selectivity in the reaction of 3-substituted
pyridine 1-oxides with phosphoryl chloride
AUTHOR(S): Yamanaka, Hiroshi; Araki, Tomio; Sakamoto, Takao
CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1988), 36(6),
2244-7
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:192171

10/583635

AB Site selectivity in the reaction of 3-substituted pyridine 1-oxides with phosphoryl chloride was investigated. When a strongly electron-withdrawing group e.g., (CN, CONRR', CO₂R, NO₂) was substituted at the 3-position, the reaction of 3-substituted pyridine 1-oxides with phosphoryl chloride yielded 3-substituted 2-chloropyridines as the main products.

CC 22-13 (Physical Organic Chemistry)
Section cross-reference(s): 29

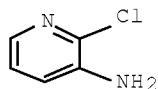
IT ~~6298-19-7~~, 3-Amino-2-chloropyridine
RL: PROC (Process)
(conversion of, to chloro(dimethylamino)pyridine)

IT 109-09-1P 626-61-9P 1452-94-4P 1681-36-3P ~~2402-77-9P~~
4548-45-2P 5470-18-8P 6602-54-6P 13091-23-1P 16110-09-1P
18368-64-4P 18368-76-8P 19069-63-7P 31557-57-0P 33252-28-7P
36953-42-1P 37831-62-2P 38029-99-1P 41288-91-9P 49608-01-7P
52200-48-3P 53939-30-3P 54864-96-9P 55675-97-3P 55934-00-4P
66600-05-3P 89284-61-7P 120234-29-9P 120234-30-2P
RL: SPN (Synthetic preparation); ~~PREF~~ (Preparation)
(preparation of)

IT ~~6298-19-7~~, 3-Amino-2-chloropyridine
RL: PROC (Process)
(conversion of, to chloro(dimethylamino)pyridine)

RN 6298-19-7 ZCAPLUS

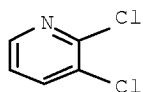
CN 3-Pyridinamine, 2-chloro- (CA INDEX NAME)



IT ~~2402-77-9P~~
RL: SPN (Synthetic preparation); ~~PREF~~ (Preparation)
(preparation of)

RN 2402-77-9 ZCAPLUS

CN Pyridine, 2,3-dichloro- (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 11:56:30 ON 06 MAR 2009)

FILE 'ZCAPLUS' ENTERED AT 11:56:38 ON 06 MAR 2009

FILE 'ZCAPLUS' ENTERED AT 11:56:54 ON 06 MAR 2009

L1 1 SEA SPE=ON ABB=ON PLU=ON US2006-583635/APPS
D SCA
SEL RN

FILE 'REGISTRY' ENTERED AT 11:57:51 ON 06 MAR 2009

L2 9 SEA SPE=ON ABB=ON PLU=ON (1317-38-0/BI OR 2402-77-9/BI OR
462-08-8/BI OR 6298-19-7/BI OR 73074-20-1/BI OR 7447-39-4/BI
OR 7632-00-0/BI OR 94770-75-9/BI OR 98-92-0/BI)

L3 1 SEA SPE=ON ABB=ON PLU=ON 2402-77-9
D SCA
D SCA L2

L4 6 SEA SPE=ON ABB=ON PLU=ON L2 AND NC5/ES
D SCA

L5 5 SEA SPE=ON ABB=ON PLU=ON L4 NOT L3

FILE 'ZCAPLUS' ENTERED AT 12:01:09 ON 06 MAR 2009

L6 23 SEA SPE=ON ABB=ON PLU=ON L3 (L) PREP/RL
L7 5 SEA SPE=ON ABB=ON PLU=ON L5 AND L6
D SCA

FILE 'REGISTRY' ENTERED AT 12:02:06 ON 06 MAR 2009

L8 1 SEA SPE=ON ABB=ON PLU=ON 2402-77-9/CRN
D SCA
SEL RN L5

L9 572 SEA SPE=ON ABB=ON PLU=ON (462-08-8/CRN OR 6298-19-7/CRN OR
73074-20-1/CRN OR 94770-75-9/CRN OR 98-92-0/CRN)

L10 2 SEA SPE=ON ABB=ON PLU=ON L8 OR L3

L11 575 SEA SPE=ON ABB=ON PLU=ON L9 OR L5

FILE 'ZCAPLUS' ENTERED AT 12:03:24 ON 06 MAR 2009

L12 23 SEA SPE=ON ABB=ON PLU=ON L10 (L) PREP/RL
L13 5 SEA SPE=ON ABB=ON PLU=ON L11 AND L12
D SCA

FILE 'REGISTRY' ENTERED AT 12:04:32 ON 06 MAR 2009

L14 544228 SEA SPE=ON ABB=ON PLU=ON CU/ELS

FILE 'ZCAPLUS' ENTERED AT 12:04:50 ON 06 MAR 2009

L15 TRA PLU=ON L13 1- RN : 99 TERMS

FILE 'REGISTRY' ENTERED AT 12:04:51 ON 06 MAR 2009

L16 99 SEA SPE=ON ABB=ON PLU=ON L15

L17 5 SEA SPE=ON ABB=ON PLU=ON L14 AND L16

L*** DEL 14673 S ?NITRIT?/BI

L18 14680 SEA SPE=ON ABB=ON PLU=ON ?NITRIT?/CNS

L19 1 SEA SPE=ON ABB=ON PLU=ON L16 AND L18
D SCA

L20 32 SEA SPE=ON ABB=ON PLU=ON L16 AND NC5/ESS AND N>1
D SCA

FILE 'ZCAPLUS' ENTERED AT 12:06:54 ON 06 MAR 2009

10/583635

L21 2 SEA SPE=ON ABB=ON PLU=ON L13 AND (L17 OR L19)
L22 3 SEA SPE=ON ABB=ON PLU=ON L13 AND (CU/BI OR COPPER?/BI OR
CUPR?/BI)

FILE 'REGISTRY' ENTERED AT 12:09:01 ON 06 MAR 2009
D SCA L3

L23 16 SEA SPE=ON ABB=ON PLU=ON C5H3CL2N/MF
D SCA

FILE 'ZCAPLUS' ENTERED AT 12:10:01 ON 06 MAR 2009

L24 163 SEA SPE=ON ABB=ON PLU=ON L23 (L) PREP/RL
L25 5 SEA SPE=ON ABB=ON PLU=ON L5 AND L24

FILE 'REGISTRY' ENTERED AT 12:11:15 ON 06 MAR 2009

SEL RN L23
L26 109 SEA SPE=ON ABB=ON PLU=ON (1001003-85-5/CRN OR 1001003-86-6/C
RN OR 1001003-87-7/CRN OR 1001003-88-8/CRN OR 1001003-91-3/CRN
OR 1001003-97-9/CRN OR 16110-09-1/CRN OR 2402-77-9/CRN OR
2402-78-0/CRN OR 2457-47-8/CRN OR 25586-45-2/CRN OR 26452-80-2/
CRN OR 55934-00-4/CRN OR 70735-32-9/CRN OR 851516-88-6/CRN OR
98136-41-5/CRN)
L27 125 SEA SPE=ON ABB=ON PLU=ON L23 OR L26
D SCA L5
SEL MF L5
L28 571 SEA SPE=ON ABB=ON PLU=ON (C5H5CLN2.CLH/MF OR C5H5CLN2/MF OR
C5H6N2.CLH/MF OR C5H6N2/MF OR C6H6N2O/MF)
L29 151 SEA SPE=ON ABB=ON PLU=ON L28 AND NC5/ES
L30 151 SEA SPE=ON ABB=ON PLU=ON L5 OR L29

FILE 'ZCAPLUS' ENTERED AT 12:13:52 ON 06 MAR 2009

L31 209 SEA SPE=ON ABB=ON PLU=ON L27 (L) PREP/RL
L32 23 SEA SPE=ON ABB=ON PLU=ON L30 AND L31

FILE 'REGISTRY' ENTERED AT 12:15:52 ON 06 MAR 2009

FILE 'ZCAPLUS' ENTERED AT 12:16:02 ON 06 MAR 2009
L33 TRA PLU=ON L32 1- RN : 7677 TERMS

FILE 'REGISTRY' ENTERED AT 12:16:07 ON 06 MAR 2009

L34 7677 SEA SPE=ON ABB=ON PLU=ON L33
L35 6 SEA SPE=ON ABB=ON PLU=ON L34 AND L14

FILE 'ZCAPLUS' ENTERED AT 12:16:58 ON 06 MAR 2009

L36 3 SEA SPE=ON ABB=ON PLU=ON L32 AND L35
L37 7 SEA SPE=ON ABB=ON PLU=ON L32 AND (CU/BI OR COPPER?/BI OR
CUPR?/BI)
D SCA
L38 9735 SEA SPE=ON ABB=ON PLU=ON L30 (L) RACT/RL
L39 3 SEA SPE=ON ABB=ON PLU=ON L38 AND L37
L40 4 SEA SPE=ON ABB=ON PLU=ON L37 NOT L39
D SCA
D SCA L39
L41 3 SEA SPE=ON ABB=ON PLU=ON L13 AND L39

FILE 'REGISTRY' ENTERED AT 12:23:58 ON 06 MAR 2009

L42 721 SEA SPE=ON ABB=ON PLU=ON L11 OR L29
L43 721 SEA SPE=ON ABB=ON PLU=ON L42 AND NC5/ES

FILE 'ZCAPLUS' ENTERED AT 12:24:31 ON 06 MAR 2009

L44 24 SEA SPE=ON ABB=ON PLU=ON L43 AND L31

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```
L45          1 SEA SPE=ON  ABB=ON  PLU=ON  L44 NOT L32
              D SCA
L46          1219793 SEA SPE=ON  ABB=ON  PLU=ON  TRANSITION?/BI
L47          0 SEA SPE=ON  ABB=ON  PLU=ON  L44 AND L46
              E COPPER+ALL/CT
L48          0 SEA SPE=ON  ABB=ON  PLU=ON  L44 AND GROUP IB/BI
L49          9 SEA SPE=ON  ABB=ON  PLU=ON  L44 AND ?DIAZ?/BI
L*** DEL     0 S L43 (L) RACT
L50          9763 SEA SPE=ON  ABB=ON  PLU=ON  L43 (L) RACT/RL
L51          5 SEA SPE=ON  ABB=ON  PLU=ON  L50 AND L31
              D SCA

FILE 'CASREACT' ENTERED AT 12:34:23 ON 06 MAR 2009
L52          STRUCTURE UPLOADED
L53          7 SEA SSS SAM L52 (    92 REACTIONS)
              D SCA
              D STAT QUE

FILE 'REGISTRY' ENTERED AT 12:35:35 ON 06 MAR 2009
L54          30743 SEA SPE=ON  ABB=ON  PLU=ON  CU/ELS AND CASREACT/LC

FILE 'CASREACT' ENTERED AT 12:35:51 ON 06 MAR 2009
L55          51052 SEA SPE=ON  ABB=ON  PLU=ON  L54
L56          0 SEA SUB=L55 SSS SAM L52 (    0 REACTIONS)
L57          12 SEA SUB=L55 SSS FUL L52 (    77 REACTIONS)
              D SCA

FILE 'ZCAPLUS' ENTERED AT 12:38:54 ON 06 MAR 2009

FILE 'CASREACT' ENTERED AT 12:39:12 ON 06 MAR 2009
              D OCC L57 1-

FILE 'ZCAPLUS' ENTERED AT 12:39:16 ON 06 MAR 2009

FILE 'CASREACT' ENTERED AT 12:39:43 ON 06 MAR 2009
              D HIT L57 4
L58          STRUCTURE UPLOADED

FILE 'CASREACT' ENTERED AT 12:41:20 ON 06 MAR 2009
L59          0 SEA SUB=L57 SSS SAM L58 (    0 REACTIONS)
L60          5 SEA SUB=L57 SSS FUL L58 (    12 REACTIONS)
              D SCA
L61          7 SEA SPE=ON  ABB=ON  PLU=ON  L57 NOT L60
              D SCA

FILE 'ZCAPLUS' ENTERED AT 12:43:15 ON 06 MAR 2009
L62          866 SEA SPE=ON  ABB=ON  PLU=ON  SHAPIRO R?/AU
L63          1 SEA SPE=ON  ABB=ON  PLU=ON  L62 AND L31
              D SCA
L64          4 SEA SPE=ON  ABB=ON  PLU=ON  (L27 OR L43) AND L62
              D SCA
              D SCA

FILE 'REGISTRY' ENTERED AT 12:46:08 ON 06 MAR 2009

FILE 'ZCAPLUS' ENTERED AT 12:46:11 ON 06 MAR 2009
              D STAT QUE L64
              D IBIB ABS HITSTR L64 1-4

FILE 'REGISTRY' ENTERED AT 12:47:00 ON 06 MAR 2009
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FILE 'ZCAPLUS' ENTERED AT 12:47:04 ON 06 MAR 2009

D STAT QUE L13

D STAT QUE L21

D STAT QUE L22

D STAT QUE L36

D STAT QUE L39

D STAT QUE L51

L65 8 SEA SPE=ON ABB=ON PLU=ON L13 OR L21 OR L22 OR L36 OR L51 OR
 L39

FILE 'CASREACT' ENTERED AT 12:47:51 ON 06 MAR 2009

D STAT QUE L60

FILE 'CASREACT, ZCAPLUS' ENTERED AT 12:48:04 ON 06 MAR 2009

L66 11 DUP REM L60 L65 (2 DUPLICATES REMOVED)

 ANSWERS '1-5' FROM FILE CASREACT

 ANSWERS '6-11' FROM FILE ZCAPLUS

FILE 'CASREACT' ENTERED AT 12:48:40 ON 06 MAR 2009

L67 5 SEA SPE=ON ABB=ON PLU=ON L55 (L) L60

D STAT QUE L67

FILE 'CASREACT, ZCAPLUS' ENTERED AT 12:49:21 ON 06 MAR 2009

L68 11 DUP REM L67 L65 (2 DUPLICATES REMOVED)

 ANSWERS '1-5' FROM FILE CASREACT

 ANSWERS '6-11' FROM FILE ZCAPLUS

D IBIB ABS HIT L68 1-5

D IBIB ABS HITIND HITSTR L68 6-11

FILE HOME

FILE ZCAPLUS

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FILE COVERS 1907 - 6 Mar 2009 VOL 150 ISS 11

FILE LAST UPDATED: 5 Mar 2009 (20090305/ED)

ZCaplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file

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provided by InfoChem.

STRUCTURE FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8
DICTIONARY FILE UPDATES: 4 MAR 2009 HIGHEST RN 1115640-24-8

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FILE CASREACT

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FILE CONTENT:1840 - 2 Mar 2009 VOL 150 ISS 10

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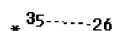
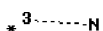
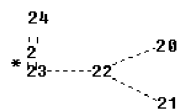
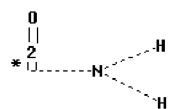
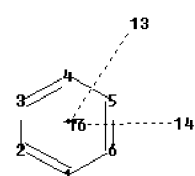
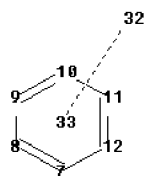
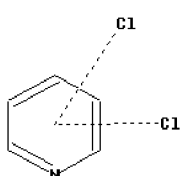
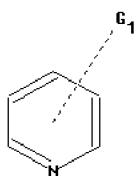
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*                                                                 *  
*      CASREACT now has more than 16.5 million reactions      *  
*                                                                 *  
*****
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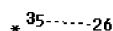
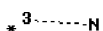
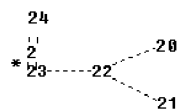
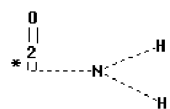
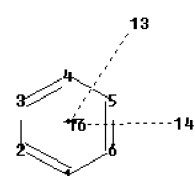
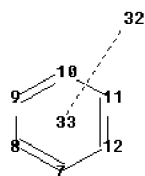
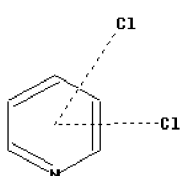
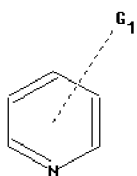
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chain nodes :
13 14 17 18 19 20 21 22 23 24 25 26 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
```

G1:[*1],[*2],[*3]

```
Connectivity :
25:2 E exact RC ring/chain 26:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 32:CLASS 33:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 7
node mappings:
1:7
```

Uploading L58.str

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```
chain nodes :
13 14 17 18 19 20 21 22 23 24 25 26 32
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
17-18 17-19 20-22 21-22 22-23 23-24 25-26
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
```

G1:[*1],[*2],[*3]

```
Connectivity :
25:2 E exact RC ring/chain 26:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 32:CLASS 33:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 7
reaction site bonds:
13-15:CC
node mappings:
1:7
```


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=>